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Evidence of Polarons and Bipolarons in a Chemically Pressurized BiAlErCCeOy: A Monte-Carlo ion Bombardment Approach

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Abstract. The polarons and bipolarons theory of superconductivity has gained so much recognition in under-doped and over-doped cuprates compound. However, the dynamics of polarons and bipolarons in both aforementioned settings is a little trivial owing to the established theories of electron-phonon interactions. In this study, we investigated the role of polarons and bipolarons in a chemically pressurized compound i.e., using Monte Carlo ion bombardment approach was 99999 ions were used in the experiment. It was observed that 4995 ions was used break the first layer of the material. The remaining 95004 ions oscillates within an equilibrium that suggest the presence of a periodic lattice i.e., in whom condensate flows without resistance. Based on this discovery it is suggested that BiAlErCCeOy may be a superconductor.

1. Introduction

Under low temperature various materials become superconductors [1-2]. A superconductor can be viewed as a Fermi liquid of electrons with a phonon-mediated mechanism between the electrons near the Fermi surface that initiates cooper pairs and the structure of the Bose-Einstein condensate. The Bose-Einstein condensate is referred as the state of matter that is composed of very large number of particles, bosons, that have the same energy level. The structure of the material is proposed to determine the dynamics of the condensates. In this light, there are many lattice modifications that have reveal different ideas of physics. Emin [3] worked on the *p*-doped La_2CuO_4 whose lattices were modified by the removal of two electrons from the out-of-plane orbitals of four oxygen ions that has been circumscribed by four copper ions of a CuO_2 layer. This type of lattice modification was to investigate the nature of bipolaron. The results shows that the oxygen dianions relax inwardly and donate electrons to the surrounding outwardly relaxing copper cations. It was proposed that this unique behaviour was as a result of charge transfer that generates a strong in-plane electron–lattice interaction that is expected to stabilise a large-bipolaron that have high susceptibility to decompose into polarons. However, there is the possibility that this lattice modification could yield two coupled condensates whose collective excitation corresponding to a relative phase oscillation i.e., a phason [4].

The dynamics of the Bose-Einstein condensate are driven by the potentials created by the lattice modification. Zheng and Gu [5] reported that condensate flows without resistance in the periodic lattice. It was proposed that as condensates flow, the effective mass of atoms is increased and enhances the nonlinearity of the imposed double-well condensate. At this state, condensate can be localized in the π-mode self-trapping regime. The evidence of self-trapping re-occurred when Zhang et al. [6] investigated the dynamics of Bose–Einstein condensate in one-dimensional driven tilted

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periodic optical lattices. The critical conditions that must be fulfilled for the transition of the condensate from diffusion to self-trapping and to soliton were controlled by constant force, the amplitude of the modulation and the phase difference within the lattice system. This result corroborated the fact that atom-atom interactions in Bose-Einstein condensates create rich and interesting nonlinear effects [7]. In under-doped cuprates material, the extrinsic and intrinsic self-trapping (ST) of charge carriers are controlled by binding energies and radii of the extrinsic and intrinsic large polarons and bipolarons in the material [8]. Therefore looking at the properties of the polarons and bipolarons as defined in Figure 1.

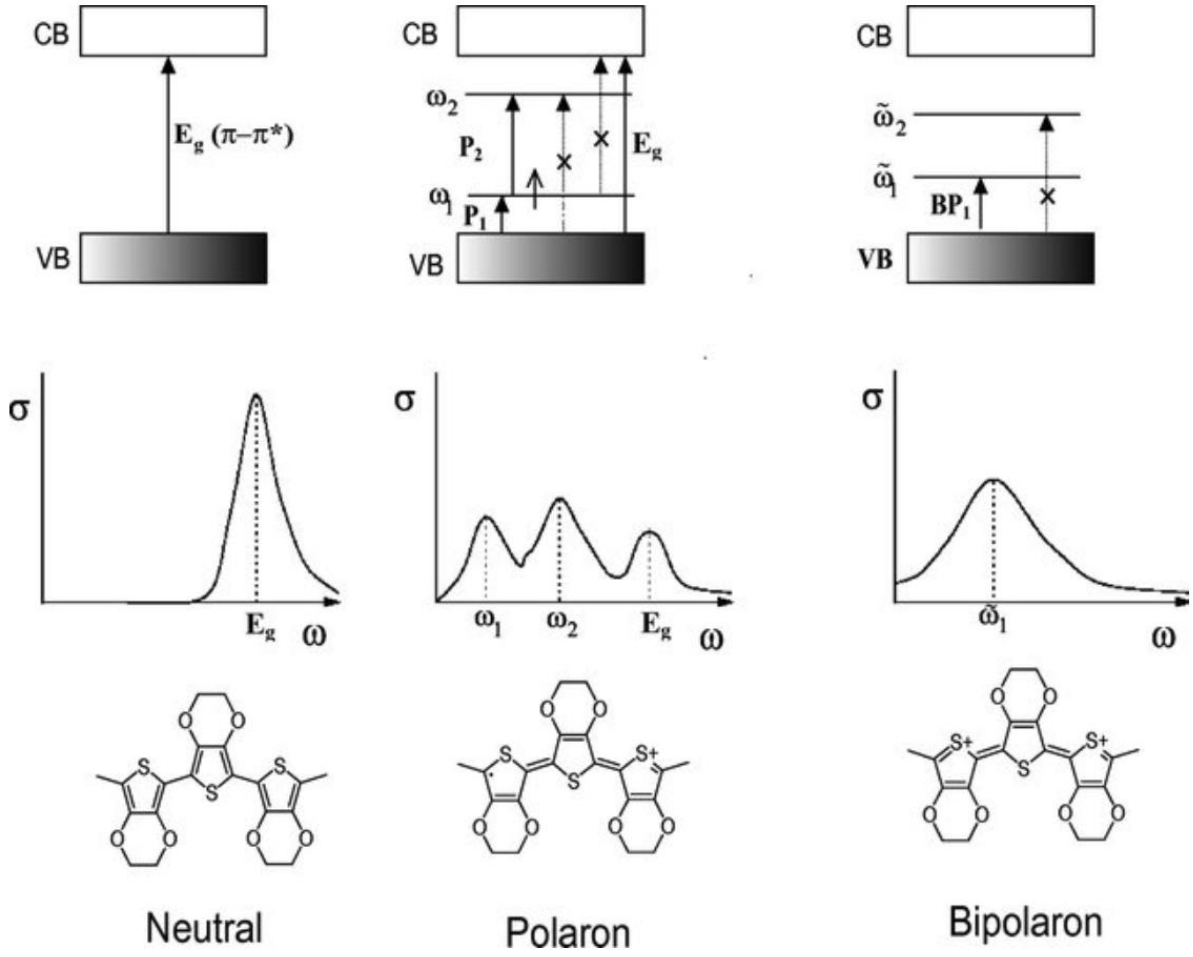

Figure 1. Nature of polaron and bipolaron [9]

Hwang et al. [9] postulated that polarons, which yields three broad peaks, is the expected state when the system is lightly doped, whereas the bipolarons, which yields only a single-broader peak is the expected state when the system is heavily doped. Hence, the difference between a neutral lattice and bipolarons lattice is the size of the peaks, i.e., broader peaks characterize bipolarons. The nature of the polarons is a three connecting narrow peaks. Based on the above, Alexandrov [10] further defined polarons and dipolarons in a strong-coupled regime. He postulated that the long-range Fröhlich electron-phonon interaction in superconducting cuprates enable carriers to be polaronic so as to form pairs. The research concluded that electronic matter in layered cuprates is charged Bose-liquid of small mobile bipolarons. Based on this polaron-bipolaron theory of superconductivity, Zhao [11] observed that underdoped cuprates are consistent with Bose-Einstein condensation of inter-site bipolarons while the overdoped cuprates still maintains the BCS-like superconductors.

In this research, we consider a chemically pressurized compound whose lattices have been modified by chemical substitution. In this case, the 'charge reservoir block' i.e. BO - $[CO]_m$ – DO (where O is oxygen, B = bismuth, C= aluminium, D=erbium) will be substituted with another element and the 'superconducting block i.e., CeO_2-$[A\text{-}CeO_2]_{k-1}$ (where A =carbon) modified in same vein. The focus of the research is to affirm the role of polarons and bipolarons in a chemically pressurized compound.

2. Methodology

Monte Carlo simulations of ion transport were performed using the Transport of ions in matter (TRIM) module of the SRIM software package [12]. TRIM calculations assume the target temperature to be absolute zero. SRIM was used because it has the ability to determine the smallest impact parameter that occurs over the path length [13]. All target atoms were stationary. The ion range in the material was taken at an angle and energy of 20^o and 2MeV respectively. The He^+ ion and its energy were adopted based on the Rutherford Backscattering experiment reported in Ref [14]. The thickness of the material was 1.68 cm. The Monte Carlo simulation of the bombardment of $BiAlErCCeO_y$ with 99,999 He^+ was performed**.** The statistics of the ion range for all 99,999 ions was partitioned and analyzed by finding the averages of 100 sections in each of 999 ions that was considered.

3. Results and Discussion

Figure 1 represents the ion distribution in the compound. The statistics of the ion distribution shows an ion range of 3653 A, skewness of -3.255, straggle of 275 A, cell width of 5 A and kurtosis of 23.277. The ion distribution shows the polarons and bipolarons in the lattices at different energies. The phonon created in lattices via the target ionization where the total ionization is given as 1969.8 keV/Ion. It was observed that the total target damage was 1.41 keV/Ion. This information show that 0.07% of the lattice is affected by the high He+ bombardment. The total phonon created is given as 28.8 keV/Ion i.e., occurs in 1.46% portion of the lattices as already described in Figure 2. Figure 3 also shows that the target ionization decreases with respect to the thickness of the material. The elemental energy budget is presented in Table 1. It is shown that under same displacement energy and lattice binding energy, the surface binding energy (SBE) varied. Carbon and Cerium had the highest SBE as presented.

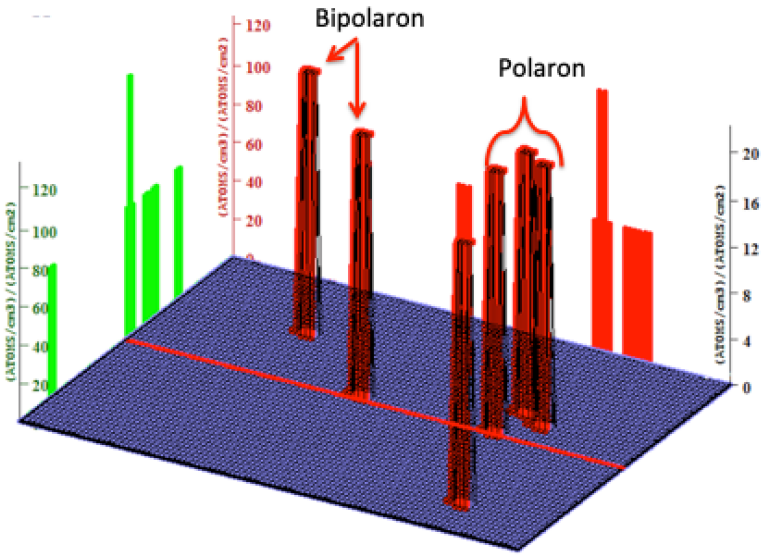

Figure 2. Ion distribution of $BiAlErCCeO_y$

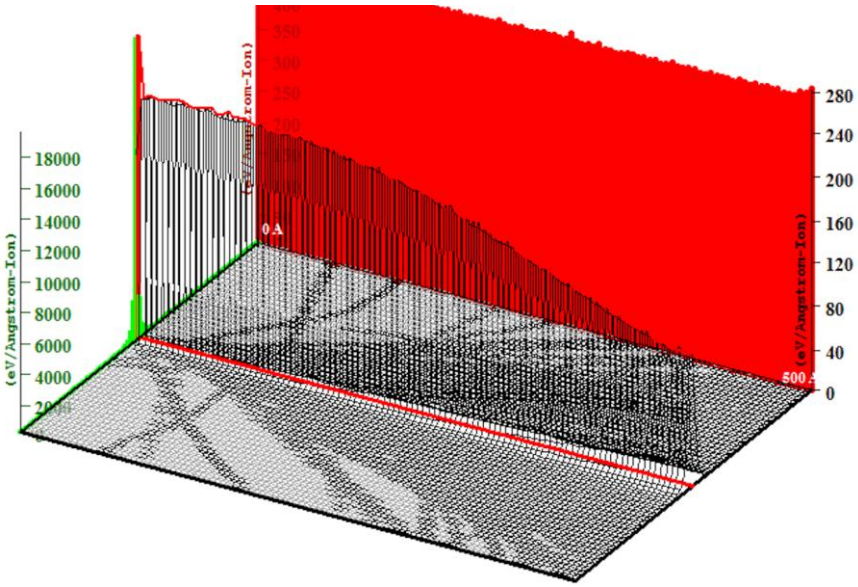

Figure 3. Target ionization of $BiAlErCCeO_y$

Table 1: Elemental energy budget

Element	Displacement Energy (eV)	Lattice Binding Energy (eV)	Surface Binding Energy (eV)
Bi	25	3	2.17
Al	25	3	3.36
Er	25	3	3.05
C	25	3	7.41
O	25	3	2.0
Ce	25	3	4.23

The surface binding energy (SBE) necessary to remove an atom from the top surface layer in vacuum during the ion sputtering process is important in estimating other parameters such as total displacements and vacancies which is given as 56 /Ion respectively. The 99,999 ions were divided into 100 and the average of each section was calculated. The averages of the depth of each section are plotted in Figure 4.

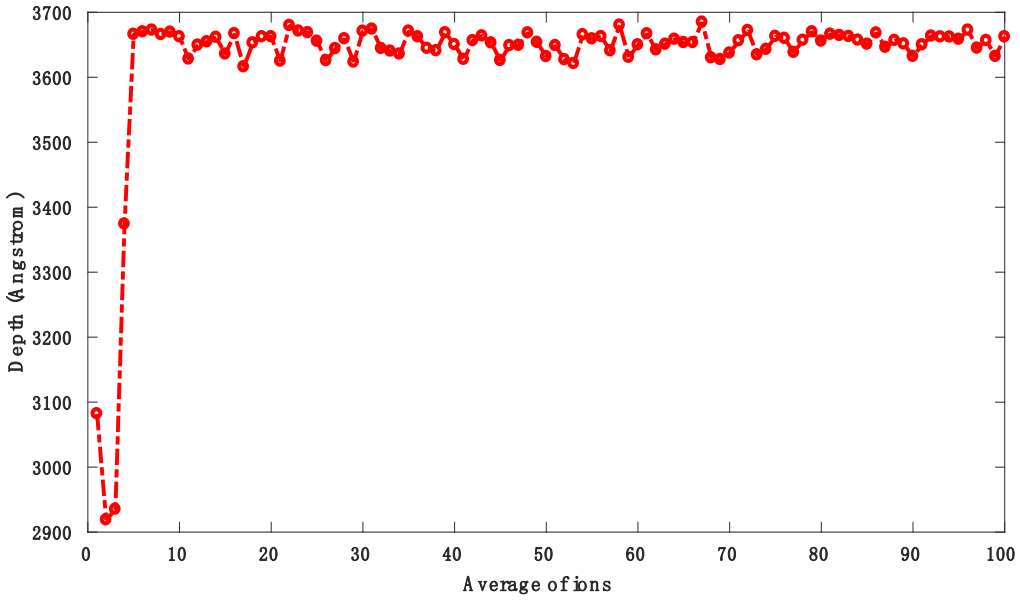

Figure 4. Depth analysis of ion bombardment

It was observed that 4995 ions was used break the first layer of the surface. The remaining 95004 ions oscillates within an equilibrium that suggest the presence of a periodic lattice i.e., in whom condensate flows without resistance [5]. This result means that at this point, It is clear that the chemically pressurized compound also had extrinsic and intrinsic self-trapping (ST) of charge carriers, which are controlled by surface binding energies and radii of the extrinsic and intrinsic large polarons and bipolarons in the material [8].

4. Conclusion

We have studied the role of poaron and bipolarons in a chemical pressurized compound. The ion bombardment technique has supported the polaron-bipolaron theory of superconductivity. This discovery may mean that BiAlErCCeOy is a superconducting material since it exhibits all the traits as seen in cuprates. The polarons and bipolarons in the chemically pressured compound is controlled by the phonons created in the lattice. The phonon was estimated to occupy 1.46% of the surface of BiAlErCCeOy. Within this lattice space, carrier localization enable the formation of extrinsic large (bi)polaronic states and intrinsic large (bi) polaronic states in the material. The surface binding energies of the individual elemental composition of the material determines the size of the polarons and bipolarons that is controlled by the carrier-phonon interactions in the lattices.

5. Acknowledgments

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